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Irreducible tensor form for the spin-photon coupling

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ABSTRACT

Using the multipole expansion of electromagnetic (EM) field, we present the spin-photon coupling in irreducible tensor form. We evaluate the matrix elements when the radiation source is described by electronic transitions in atomic systems. The results indicate that the energy corrections increase for short wavelengths and large charge number.

1. Introduction

In consequence of their results on the time-dependent Foldy–Wouthuysen transformation [1], Mondal et al. show [2] that the spin-photon coupling represents the $O(c^{-2})$ correction to the Dirac operator for an electron in a potential V and interacting with the EM field, which is characterized by the 4-component vector potential (Φ, A) (for an alternative derivation we refer to [3]):

$$H_{\mathrm{AME}} = \frac{1}{2c^2}(H^{\mathrm{in}}_{\mathrm{AME}} + H^{\mathrm{ex}}_{\mathrm{AME}}) \tag{1.1}$$

where

$$H^{\mathrm{in}}_{\mathrm{AME}} = S\cdot(E^{\mathrm{in}}\times A)\,, \quad E^{\mathrm{in}} = -\operatorname{grad} V\,, \tag{1.2a}$$

$$H^{\mathrm{ex}}_{\mathrm{AME}} = S\cdot(E^{\mathrm{ex}}\times A)\,, \quad E^{\mathrm{ex}} = -\dot{A} - \operatorname{grad}\Phi \tag{1.2b}$$

and S is the spin operator. Throughout we use atomic units unless explicitly stated otherwise. Following [2,4], the spin-photon coupling described by H_{AME} is further referred to as the angular magnetoelectric (AME) coupling. One calls $H^{\mathrm{in}}_{\mathrm{AME}}$ (resp. $H^{\mathrm{ex}}_{\mathrm{AME}}$) an intrinsic (resp. induced) part of AME coupling. In the Coulomb gauge fixing, $H^{\mathrm{ex}}_{\mathrm{AME}}$ serves as the source for obtaining the "hidden energy" that couples the EM angular momentum density with magnetic moments [4].

It is our purpose here to investigate the influence of H_{AME} on the atomic energy levels provided that the radiation source is defined by electronic transitions. The exploration of the standard multipole expansion of EM field [5] allows us to represent H_{AME} as the summable series (in the sense of distributions) of irreducible tensor operators, while the information about the radiation source is contained separately, in the coefficients of expansion (amplitudes).

As one could expect, the contribution of the AME coupling to the total energy should be small enough. For example, we show that the matrix elements of the intrinsic part are of order $O(\omega^2 Z^2 c^{-3})$ for the $E1$ transition, while the matrix elements of the induced part are of order $O(\omega^5 Z^{-2} c^{-6})$ for the same type of radiation; here ω is the transition energy. However, ω usually increases as the charge number Z becomes large, which results in larger energy corrections.

By (1.2), $H^{\mathrm{in}}_{\mathrm{AME}}$ is time-dependent, while $H^{\mathrm{ex}}_{\mathrm{AME}}$ is time-independent. The latter is in agreement with [2], where the plane EM wave expansion is used for explaining the inverse Faraday effect. In addition, we show that $H^{\mathrm{ex}}_{\mathrm{AME}}$ can be split in two separate parts. One part is traditional in the sense that it does not vanish if the multipole moment of order $l \in \mathbb{N}$ is nonzero for at least one fixed l, while the second one is more "exotic" in the sense that it can be nonzero only if the multipole moment is nonzero for at least two different l. The latter case arises when, for example, one considers electronic satellite transitions produced by electron capture and subsequent radiative decay [6–10].

In Sec. 2 we express (1.2) in irreducible tensor form. We work in the Coulomb gauge fixing and we use the standard technique of angular momentum theory [11–14] (including the notation and the phase system used therein). We discuss the matrix elements in particular cases in Sec. 3.

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2. Tensor operators

2.1. Amplitudes

Let the radiation of energy $\omega = \nu c = E_{\alpha J} - E_{\alpha' J'}$ be emitted by the electron going from the state $|\alpha JM\rangle$ to the (lower) state $|\alpha' J' M'\rangle$; α and α' denote additional quantum numbers if necessary. When $\nu \ll 1$, the amplitudes for the radiation of order (l, m), $l \in \mathbb{N}$, $m \in \{-l, \ldots, l\}$, are approximated by [5]

$$a^{\#}_{\nu lm} = \delta_{m\rho} a^{\#}_{\nu l}, \quad \rho = M - M'. \tag{2.1}$$

Here the superscript denotes both E (electric type) and M (magnetic type), and

$$a^{\mathrm{E}}_{\nu l} = \lambda_{\nu l} Q_{\nu l}, \quad a^{\mathrm{M}}_{\nu l} = -\lambda_{\nu l} M_{\nu l}. \tag{2.2}$$

The multiplier $\lambda_{\nu l}$ is given by

$$\begin{aligned}\lambda_{\nu l} =& (-1)^{J-J'+1} \frac{\mathrm{i}^{-l} \nu^{l+2} K_l}{(2l+1)!!} \frac{\sqrt{4\pi(2l+1)}}{\sqrt{2J+1}} \\ & \cdot \begin{bmatrix} J' & l & J \\ M' & \rho & M \end{bmatrix}, \quad K_l = -\sqrt{1 + 1/l}.\end{aligned} \tag{2.3}$$

The number $Q_{\nu l}$ (resp. $M_{\nu l}$) is the reduced matrix element of the electric (resp. magnetic) multipole moment Q^l (resp. M^l):

$$Q_{\nu l} = (\alpha' J' \| Q^l \| \alpha J), \quad M_{\nu l} = (\alpha' J' \| M^l \| \alpha J). \tag{2.4}$$

When the magnetization is ignored, we have

$$Q^l = -r^l C^l, \quad M^l = -\frac{\sqrt{l(2l-1)}}{c(l+1)} r^{l-1} [C^{l-1} \times L^1]^l. \tag{2.5}$$

Otherwise: Q^l is replaced by $Q^l + O(\nu/c)$, hence we omit the $O(\nu/c)$ correction since we already have the small ν^{l+2} in (2.3); M^l is replaced by $M^l + M'^l$, where

$$M'^l = -\frac{1}{c} \sqrt{l(2l-1)} r^{l-1} [C^{l-1} \times S^1]^l. \tag{2.6}$$

In the examples to be followed, we assume $M^l + M'^l$ when we write M^l; see also [11, Secs. 4 and 25].

2.2. Intrinsic part

As in [2], we take the real part of the external electric field E^{ex}. Applying the well-known angular momentum technique, we deduce from [5, Appendix B.2] the following form for the intrinsic part $H^{\mathrm{in}}_{\mathrm{AME}} \equiv (H^{\mathrm{in}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu t}$ of electric type

$$(H^{\mathrm{in}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu t} = \sum_{l \in \mathbb{N}} \sum_{m=-l}^{l} \alpha^{\mathrm{E}}_{\nu lm}(t) (H^{\mathrm{in}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu lm} \tag{2.7a}$$

where the rank-l irreducible tensor operator is

$$\begin{aligned}(H^{\mathrm{in}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu l} =& \frac{\mathrm{i}^{-l} V'(r)}{2\omega\sqrt{\pi(2l+1)}} [C^l \times S^1]^l \\ & \cdot [(l+1) j_{l-1}(\nu r) - l j_{l+1}(\nu r)]\end{aligned} \tag{2.7b}$$

(j_l is the spherical Bessel function) and the amplitude is

$$\alpha^{\mathrm{E}}_{\nu lm}(t) = \frac{1}{2} \left(\mathrm{e}^{-\mathrm{i}(\omega t + \sigma_l)} a^{\mathrm{E}}_{\nu lm} + (-1)^m \mathrm{e}^{\mathrm{i}(\omega t + \sigma_l)} \overline{a^{\mathrm{E}}_{\nu l,-m}} \right). \tag{2.7c}$$

Here $\sigma_l = \arg \Gamma(l + 1 + \mathrm{i}\eta)$ is the Coulomb phase shift, $\eta = -Z/\nu$ is the Sommerfeld parameter.

Likewise, the intrinsic part $H^{\mathrm{in}}_{\mathrm{AME}} \equiv (H^{\mathrm{in}}_{\mathrm{AME}})^{\mathrm{M}}_{\nu t}$ of magnetic type is written in the form (2.7a), but with the superscript E replaced by the superscript M, and with the amplitude replaced by

$$\beta^{\mathrm{M}}_{\nu lm}(t) = \frac{1}{2} \left(\mathrm{e}^{-\mathrm{i}(\omega t + \sigma_l)} a^{\mathrm{M}}_{\nu lm} - (-1)^m \mathrm{e}^{\mathrm{i}(\omega t + \sigma_l)} \overline{a^{\mathrm{M}}_{\nu l,-m}} \right). \tag{2.8a}$$

The corresponding rank-l irreducible tensor operator is

$$\begin{aligned}(H^{\mathrm{in}}_{\mathrm{AME}})^{\mathrm{M}}_{\nu l} =& \frac{\mathrm{i}^{-l-1} V'(r) j_l(\nu r)}{2\omega\sqrt{\pi(2l+1)}} \\ & \cdot \left(\sqrt{(l+1)(2l-1)} [C^{l-1} \times S^1]^l \right. \\ & \left. - \sqrt{l(2l+3)} [C^{l+1} \times S^1]^l \right).\end{aligned} \tag{2.8b}$$

In [2] the authors put $A = B \times x/2$ for almost every $x \in \mathbb{R}^3$. In this case $\operatorname{div} A^{\mathrm{M}} = 0$ but $\operatorname{div} A^{\mathrm{E}} \neq 0$; for $A = A^{\mathrm{M}}$ of magnetic type, $j_l(\nu r)$ in (2.8b) is replaced by $[(l+2) j_l(\nu r) - \nu r j_{l+1}(\nu r)]/2$.

From the point of view of energy levels, the treatment of $H^{\mathrm{in}}_{\mathrm{AME}}/(2c^2)$, when considered as the $O(c^{-2})$ correction to the Pauli operator for an electron in a potential V, is subtle in that it is time-dependent. We refer to [15–17], where the eigenvalue problem for the time-dependent Pauli equation is studied in detail.

2.3. Induced part

Unlike the intrinsic part of AME coupling, the induced part contains the products of the time-dependent amplitudes $\alpha^{\#}_{\nu lm}(t)$ and $\beta^{\#}_{\nu l'm'}(t)$; here $\alpha^{\mathrm{M}}_{\nu lm}(t)$ (resp. $\beta^{\mathrm{E}}_{\nu lm}(t)$) is defined by (2.7c) (resp. (2.8a)), but with the superscript E (resp. M) replaced by the superscript M (resp. E). However, using the symmetry properties of the products and interchanging the summation indices l and l' we find that the induced part of AME coupling is actually time-independent. As a result, $H^{\mathrm{ex}}_{\mathrm{AME}} \equiv (H^{\mathrm{ex}}_{\mathrm{AME}})^{\#}_{\nu}$ splits into two parts:

$$(H^{\mathrm{ex}}_{\mathrm{AME}})^{\#}_{\nu} = (H^{\mathrm{ex}}_{\mathrm{AME}})^{\#\prime}_{\nu} + (H^{\mathrm{ex}}_{\mathrm{AME}})^{\#\prime\prime}_{\nu}. \tag{2.9}$$

For the radiation of electric type we have

$$\begin{aligned}(H^{\mathrm{ex}}_{\mathrm{AME}})^{\mathrm{E}\prime}_{\nu} =& \frac{(-1)^\rho}{2} \sum_l |a^{\mathrm{E}}_{\nu l}|^2 \\ & \cdot \sum_{J = \mathrm{odd}} (H^{\mathrm{ex}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu ll J0} \begin{bmatrix} l & l & J \\ \rho & -\rho & 0 \end{bmatrix},\end{aligned} \tag{2.10a}$$

$$\begin{aligned}(H^{\mathrm{ex}}_{\mathrm{AME}})^{\mathrm{E}\prime\prime}_{\nu} =& (-1)^\rho \sum_{l<l'} \sum_J \gamma^{\mathrm{E}}_{\nu ll'J} (H^{\mathrm{ex}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu ll'J0} \\ & \cdot \begin{bmatrix} l & l' & J \\ \rho & -\rho & 0 \end{bmatrix}\end{aligned} \tag{2.10b}$$

with $l \geq \max\{1, |\rho|\}$. The "amplitude" is

$$\gamma^{\mathrm{E}}_{\nu ll'J} = \frac{1}{2} \left(\mathrm{e}^{-\mathrm{i}(\sigma_l - \sigma_{l'})} a^{\mathrm{E}}_{\nu l} \overline{a^{\mathrm{E}}_{\nu l'}} - (-1)^{l+l'+J} \mathrm{e}^{\mathrm{i}(\sigma_l - \sigma_{l'})} \overline{a^{\mathrm{E}}_{\nu l}} a^{\mathrm{E}}_{\nu l'} \right) \tag{2.11}$$

and $(H^{\mathrm{ex}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu ll'J0}$ is the 0th component of the rank-J ($|l - l'| \leq J \leq l + l'$) tensor operator

$$\begin{aligned}(H^{\mathrm{ex}}_{\mathrm{AME}})^{\mathrm{E}}_{\nu ll'J} =& \frac{\sqrt{3/2}\,\mathrm{i}}{2\pi\omega} (-1)^{J+1} \sum_k \mathrm{i}^k \sqrt{2k+1} [C^k \times S^1]^J \\ & \cdot \left(\sqrt{l(2l+3) l'(2l'+3)} j_{l+1}(\nu r) j_{l'+1}(\nu r) \right. \\ & \cdot \begin{bmatrix} l+1 & l'+1 & k \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} l & 1 & l+1 \\ l' & 1 & l'+1 \\ J & 1 & k \end{Bmatrix} \\ & - \sqrt{l(2l+3)(l'+1)(2l'-1)} j_{l+1}(\nu r) j_{l'-1}(\nu r) \\ & \cdot \begin{bmatrix} l+1 & l'-1 & k \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} l & 1 & l+1 \\ l' & 1 & l'-1 \\ J & 1 & k \end{Bmatrix} \\ & - \sqrt{(l+1)(2l-1) l'(2l'+3)} j_{l-1}(\nu r) j_{l'+1}(\nu r)\end{aligned}$$

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